



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 10:00 am BST

PDB ID : 5OCD
Title : structure of a CDPS from *Fluoribacter dumoffii*
Authors : Schmitt, E.; Mechulam, Y.; Bourgeois, G.
Deposited on : 2017-06-30
Resolution : 3.06 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

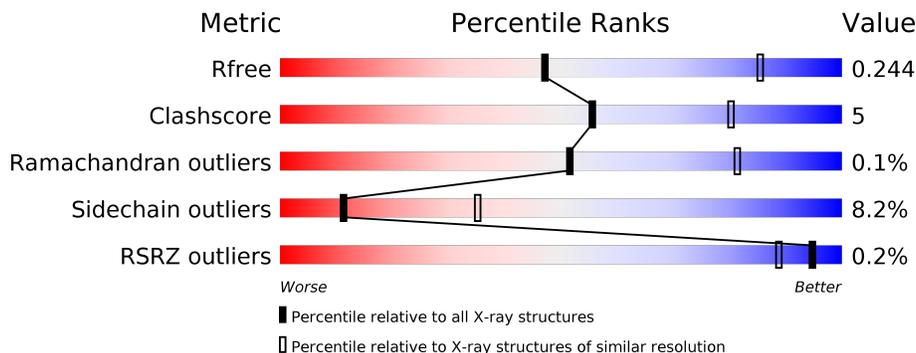
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.06 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	266	 67% 16% 15%
1	B	266	 70% 13% 15%
1	C	266	 71% 11% 15%
1	D	266	 71% 12% 15%
1	E	266	 67% 16% 16%
1	F	266	 64% 16% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	266	 67% 14% 17%
1	H	266	 69% 15% 15%
1	I	266	 71% 11% 16%
1	J	266	 69% 13% 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18821 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cyclodipeptide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	226	1893	1212	329	342	10	0	0	0
1	B	226	1893	1212	329	342	10	0	0	0
1	C	226	1892	1213	328	341	10	0	0	0
1	D	225	1885	1208	327	340	10	0	0	0
1	E	224	1880	1204	327	339	10	0	0	0
1	F	220	1842	1181	319	332	10	0	0	0
1	G	221	1846	1184	317	335	10	0	0	0
1	H	226	1886	1210	325	341	10	0	0	0
1	I	224	1874	1202	323	339	10	0	0	0
1	J	224	1874	1202	323	339	10	0	0	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A0W0T5C6
A	1	ALA	-	expression tag	UNP A0A0W0T5C6
A	258	SER	-	expression tag	UNP A0A0W0T5C6
A	259	ARG	-	expression tag	UNP A0A0W0T5C6
A	260	HIS	-	expression tag	UNP A0A0W0T5C6
A	261	HIS	-	expression tag	UNP A0A0W0T5C6
A	262	HIS	-	expression tag	UNP A0A0W0T5C6
A	263	HIS	-	expression tag	UNP A0A0W0T5C6
A	264	HIS	-	expression tag	UNP A0A0W0T5C6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	HIS	-	expression tag	UNP A0A0W0T5C6
B	0	MET	-	initiating methionine	UNP A0A0W0T5C6
B	1	ALA	-	expression tag	UNP A0A0W0T5C6
B	258	SER	-	expression tag	UNP A0A0W0T5C6
B	259	ARG	-	expression tag	UNP A0A0W0T5C6
B	260	HIS	-	expression tag	UNP A0A0W0T5C6
B	261	HIS	-	expression tag	UNP A0A0W0T5C6
B	262	HIS	-	expression tag	UNP A0A0W0T5C6
B	263	HIS	-	expression tag	UNP A0A0W0T5C6
B	264	HIS	-	expression tag	UNP A0A0W0T5C6
B	265	HIS	-	expression tag	UNP A0A0W0T5C6
C	0	MET	-	initiating methionine	UNP A0A0W0T5C6
C	1	ALA	-	expression tag	UNP A0A0W0T5C6
C	258	SER	-	expression tag	UNP A0A0W0T5C6
C	259	ARG	-	expression tag	UNP A0A0W0T5C6
C	260	HIS	-	expression tag	UNP A0A0W0T5C6
C	261	HIS	-	expression tag	UNP A0A0W0T5C6
C	262	HIS	-	expression tag	UNP A0A0W0T5C6
C	263	HIS	-	expression tag	UNP A0A0W0T5C6
C	264	HIS	-	expression tag	UNP A0A0W0T5C6
C	265	HIS	-	expression tag	UNP A0A0W0T5C6
D	0	MET	-	initiating methionine	UNP A0A0W0T5C6
D	1	ALA	-	expression tag	UNP A0A0W0T5C6
D	258	SER	-	expression tag	UNP A0A0W0T5C6
D	259	ARG	-	expression tag	UNP A0A0W0T5C6
D	260	HIS	-	expression tag	UNP A0A0W0T5C6
D	261	HIS	-	expression tag	UNP A0A0W0T5C6
D	262	HIS	-	expression tag	UNP A0A0W0T5C6
D	263	HIS	-	expression tag	UNP A0A0W0T5C6
D	264	HIS	-	expression tag	UNP A0A0W0T5C6
D	265	HIS	-	expression tag	UNP A0A0W0T5C6
E	0	MET	-	initiating methionine	UNP A0A0W0T5C6
E	1	ALA	-	expression tag	UNP A0A0W0T5C6
E	258	SER	-	expression tag	UNP A0A0W0T5C6
E	259	ARG	-	expression tag	UNP A0A0W0T5C6
E	260	HIS	-	expression tag	UNP A0A0W0T5C6
E	261	HIS	-	expression tag	UNP A0A0W0T5C6
E	262	HIS	-	expression tag	UNP A0A0W0T5C6
E	263	HIS	-	expression tag	UNP A0A0W0T5C6
E	264	HIS	-	expression tag	UNP A0A0W0T5C6
E	265	HIS	-	expression tag	UNP A0A0W0T5C6
F	0	MET	-	initiating methionine	UNP A0A0W0T5C6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	ALA	-	expression tag	UNP A0A0W0T5C6
F	258	SER	-	expression tag	UNP A0A0W0T5C6
F	259	ARG	-	expression tag	UNP A0A0W0T5C6
F	260	HIS	-	expression tag	UNP A0A0W0T5C6
F	261	HIS	-	expression tag	UNP A0A0W0T5C6
F	262	HIS	-	expression tag	UNP A0A0W0T5C6
F	263	HIS	-	expression tag	UNP A0A0W0T5C6
F	264	HIS	-	expression tag	UNP A0A0W0T5C6
F	265	HIS	-	expression tag	UNP A0A0W0T5C6
G	0	MET	-	initiating methionine	UNP A0A0W0T5C6
G	1	ALA	-	expression tag	UNP A0A0W0T5C6
G	258	SER	-	expression tag	UNP A0A0W0T5C6
G	259	ARG	-	expression tag	UNP A0A0W0T5C6
G	260	HIS	-	expression tag	UNP A0A0W0T5C6
G	261	HIS	-	expression tag	UNP A0A0W0T5C6
G	262	HIS	-	expression tag	UNP A0A0W0T5C6
G	263	HIS	-	expression tag	UNP A0A0W0T5C6
G	264	HIS	-	expression tag	UNP A0A0W0T5C6
G	265	HIS	-	expression tag	UNP A0A0W0T5C6
H	0	MET	-	initiating methionine	UNP A0A0W0T5C6
H	1	ALA	-	expression tag	UNP A0A0W0T5C6
H	258	SER	-	expression tag	UNP A0A0W0T5C6
H	259	ARG	-	expression tag	UNP A0A0W0T5C6
H	260	HIS	-	expression tag	UNP A0A0W0T5C6
H	261	HIS	-	expression tag	UNP A0A0W0T5C6
H	262	HIS	-	expression tag	UNP A0A0W0T5C6
H	263	HIS	-	expression tag	UNP A0A0W0T5C6
H	264	HIS	-	expression tag	UNP A0A0W0T5C6
H	265	HIS	-	expression tag	UNP A0A0W0T5C6
I	0	MET	-	initiating methionine	UNP A0A0W0T5C6
I	1	ALA	-	expression tag	UNP A0A0W0T5C6
I	258	SER	-	expression tag	UNP A0A0W0T5C6
I	259	ARG	-	expression tag	UNP A0A0W0T5C6
I	260	HIS	-	expression tag	UNP A0A0W0T5C6
I	261	HIS	-	expression tag	UNP A0A0W0T5C6
I	262	HIS	-	expression tag	UNP A0A0W0T5C6
I	263	HIS	-	expression tag	UNP A0A0W0T5C6
I	264	HIS	-	expression tag	UNP A0A0W0T5C6
I	265	HIS	-	expression tag	UNP A0A0W0T5C6
J	0	MET	-	initiating methionine	UNP A0A0W0T5C6
J	1	ALA	-	expression tag	UNP A0A0W0T5C6
J	258	SER	-	expression tag	UNP A0A0W0T5C6

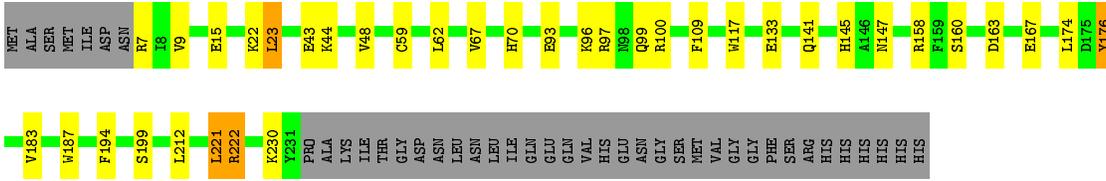
Continued on next page...

Continued from previous page...

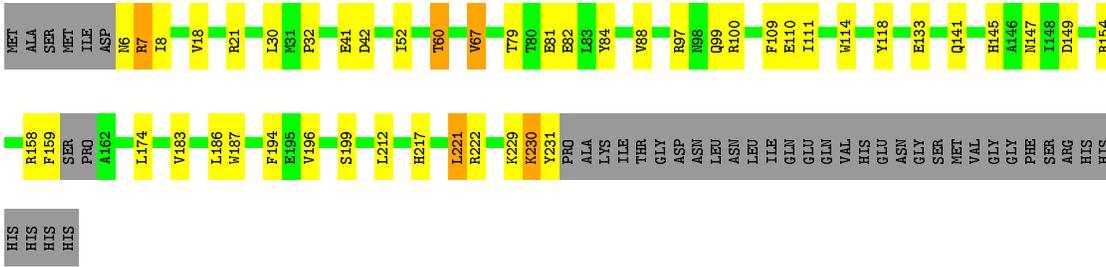
Chain	Residue	Modelled	Actual	Comment	Reference
J	259	ARG	-	expression tag	UNP A0A0W0T5C6
J	260	HIS	-	expression tag	UNP A0A0W0T5C6
J	261	HIS	-	expression tag	UNP A0A0W0T5C6
J	262	HIS	-	expression tag	UNP A0A0W0T5C6
J	263	HIS	-	expression tag	UNP A0A0W0T5C6
J	264	HIS	-	expression tag	UNP A0A0W0T5C6
J	265	HIS	-	expression tag	UNP A0A0W0T5C6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	15	Total O 15 15	0	0
2	B	8	Total O 8 8	0	0
2	C	5	Total O 5 5	0	0
2	D	9	Total O 9 9	0	0
2	E	1	Total O 1 1	0	0
2	F	1	Total O 1 1	0	0
2	G	1	Total O 1 1	0	0
2	H	4	Total O 4 4	0	0
2	I	5	Total O 5 5	0	0
2	J	7	Total O 7 7	0	0



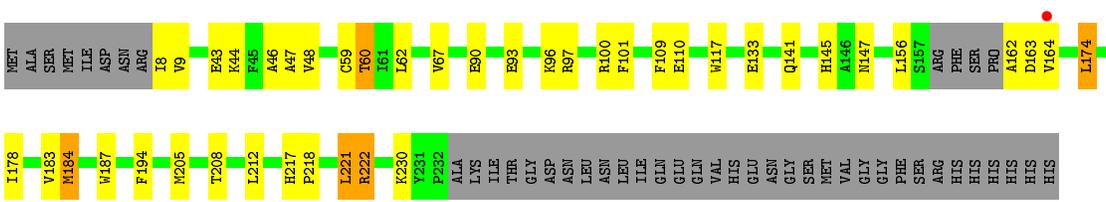
• Molecule 1: Cyclodi-peptide synthase



• Molecule 1: Cyclodi-peptide synthase



• Molecule 1: Cyclodi-peptide synthase



• Molecule 1: Cyclodi-peptide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.03Å 97.80Å 211.28Å 90.00° 115.58° 90.00°	Depositor
Resolution (Å)	48.16 – 3.06 48.16 – 3.06	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.16-3.06) 99.3 (48.16-3.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.07Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.210 , 0.249 0.217 , 0.244	Depositor DCC
R_{free} test set	3223 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	76.6	Xtrriage
Anisotropy	0.894	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18821	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5771e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	0/1943	0.73	0/2629
1	B	0.56	0/1943	0.74	0/2629
1	C	0.51	0/1943	0.70	0/2630
1	D	0.53	0/1935	0.70	0/2618
1	E	0.54	0/1928	0.71	0/2606
1	F	0.50	0/1890	0.71	0/2555
1	G	0.49	0/1894	0.72	0/2563
1	H	0.49	0/1937	0.71	0/2623
1	I	0.49	0/1924	0.70	0/2604
1	J	0.52	0/1924	0.72	0/2604
All	All	0.52	0/19261	0.71	0/26061

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1893	0	1848	21	0
1	B	1893	0	1848	18	0
1	C	1892	0	1849	19	0
1	D	1885	0	1842	14	0
1	E	1880	0	1835	20	0
1	F	1842	0	1801	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1846	0	1801	23	0
1	H	1886	0	1841	20	0
1	I	1874	0	1829	16	0
1	J	1874	0	1829	17	0
2	A	15	0	0	0	0
2	B	8	0	0	0	0
2	C	5	0	0	0	0
2	D	9	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	1	0
2	H	4	0	0	0	0
2	I	5	0	0	0	0
2	J	7	0	0	0	0
All	All	18821	0	18323	189	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 189 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ARG:HH21	1:C:222:ARG:HG3	1.24	1.03
1:D:222:ARG:HG3	1:D:222:ARG:HH21	1.24	1.02
1:J:222:ARG:HG3	1:J:222:ARG:HH21	1.25	1.01
1:G:222:ARG:HG3	1:G:222:ARG:HH21	1.26	1.01
1:F:222:ARG:HG3	1:F:222:ARG:HH21	1.26	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/266 (84%)	216 (96%)	8 (4%)	0	100	100
1	B	224/266 (84%)	218 (97%)	6 (3%)	0	100	100
1	C	224/266 (84%)	216 (96%)	8 (4%)	0	100	100
1	D	223/266 (84%)	216 (97%)	7 (3%)	0	100	100
1	E	220/266 (83%)	210 (96%)	9 (4%)	1 (0%)	29	60
1	F	216/266 (81%)	208 (96%)	7 (3%)	1 (0%)	29	60
1	G	217/266 (82%)	205 (94%)	12 (6%)	0	100	100
1	H	224/266 (84%)	215 (96%)	9 (4%)	0	100	100
1	I	222/266 (84%)	214 (96%)	8 (4%)	0	100	100
1	J	222/266 (84%)	215 (97%)	7 (3%)	0	100	100
All	All	2216/2660 (83%)	2133 (96%)	81 (4%)	2 (0%)	51	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	42	ASP
1	E	42	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/240 (86%)	185 (90%)	21 (10%)	7	24
1	B	206/240 (86%)	190 (92%)	16 (8%)	12	37
1	C	206/240 (86%)	191 (93%)	15 (7%)	14	40
1	D	205/240 (85%)	188 (92%)	17 (8%)	11	35
1	E	204/240 (85%)	187 (92%)	17 (8%)	11	35
1	F	201/240 (84%)	181 (90%)	20 (10%)	7	25
1	G	201/240 (84%)	190 (94%)	11 (6%)	21	50
1	H	205/240 (85%)	189 (92%)	16 (8%)	12	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	204/240 (85%)	189 (93%)	15 (7%)	13	39
1	J	204/240 (85%)	185 (91%)	19 (9%)	9	29
All	All	2042/2400 (85%)	1875 (92%)	167 (8%)	11	35

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	147	ASN
1	F	97	ARG
1	J	99	GLN
1	E	154	ARG
1	E	229	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	226/266 (84%)	-0.16	0 100 100	52, 70, 98, 126	0
1	B	226/266 (84%)	-0.16	0 100 100	49, 69, 102, 135	0
1	C	226/266 (84%)	-0.07	0 100 100	64, 91, 126, 153	0
1	D	225/266 (84%)	-0.10	0 100 100	60, 89, 120, 149	0
1	E	224/266 (84%)	-0.18	0 100 100	65, 95, 130, 160	0
1	F	220/266 (82%)	-0.09	0 100 100	66, 103, 144, 173	0
1	G	221/266 (83%)	-0.06	1 (0%) 91 79	70, 103, 144, 164	0
1	H	226/266 (84%)	-0.10	0 100 100	73, 97, 122, 139	0
1	I	224/266 (84%)	-0.06	0 100 100	76, 100, 123, 129	0
1	J	224/266 (84%)	-0.11	3 (1%) 77 56	60, 98, 139, 150	0
All	All	2242/2660 (84%)	-0.11	4 (0%) 95 89	49, 93, 130, 173	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	159	PHE	3.4
1	J	156	LEU	2.3
1	G	164	VAL	2.1
1	J	212	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.